



wwPDB EM Validation Summary Report ⓘ

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PDB ID : 8YUV
EMDB ID : EMD-39584
Title : Cryo-EM structure of the immepip-bound H3R-Gi complex
Authors : Shen, Q.; Tang, X.; Wen, X.; Cheng, S.; Xiao, P.; Zang, S.; Shen, D.; Jiang, L.; Zheng, Y.; Zhang, H.; Xu, H.; Mao, C.; Zhang, M.; Hu, W.; Sun, J.; Chen, Z.; Zhang, Y.
Deposited on : 2024-03-27
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

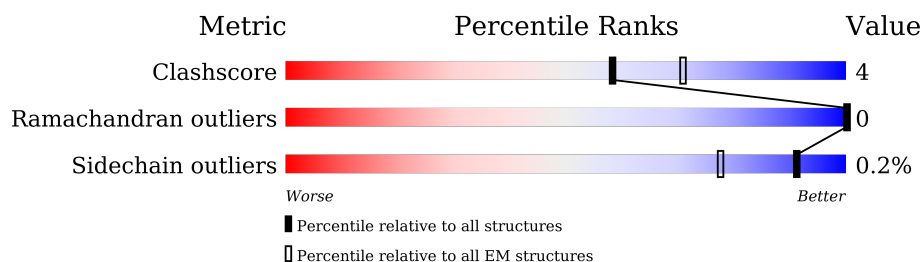
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	354	
2	B	358	
3	G	71	
4	S	269	
5	R	461	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9102 atoms, of which 61 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1811	1150	301	346	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	339	Total	C	N	O	S	0	0
			2607	1607	468	511	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	58	Total	C	N	O	S	0	0
			444	277	79	85	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	234	Total	C	N	O	S	0	0
			1795	1137	297	351	10		

- Molecule 5 is a protein called Histamine H3 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	289	Total	C	N	O	S	0	0
			2344	1559	389	384	12		

There are 16 discrepancies between the modelled and reference sequences:

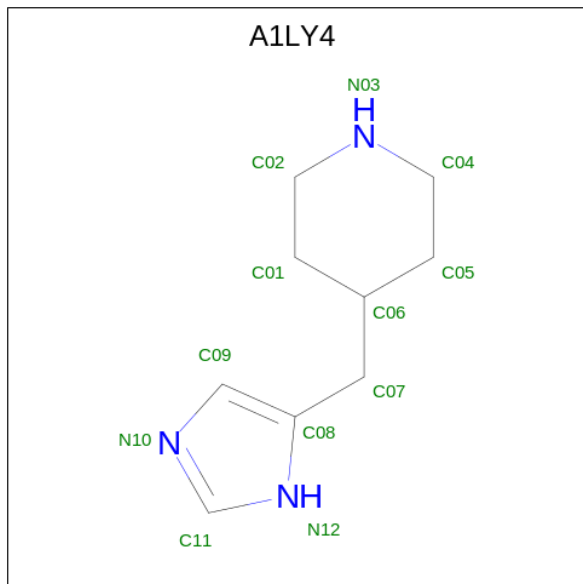
Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	ASP	-	expression tag	UNP Q9Y5N1
R	-14	TYR	-	expression tag	UNP Q9Y5N1
R	-13	LYS	-	expression tag	UNP Q9Y5N1
R	-12	ASP	-	expression tag	UNP Q9Y5N1
R	-11	ASP	-	expression tag	UNP Q9Y5N1
R	-10	ASP	-	expression tag	UNP Q9Y5N1
R	-9	ASP	-	expression tag	UNP Q9Y5N1
R	-8	LYS	-	expression tag	UNP Q9Y5N1
R	-7	LEU	-	expression tag	UNP Q9Y5N1
R	-6	GLU	-	expression tag	UNP Q9Y5N1
R	-5	VAL	-	expression tag	UNP Q9Y5N1
R	-4	LEU	-	expression tag	UNP Q9Y5N1

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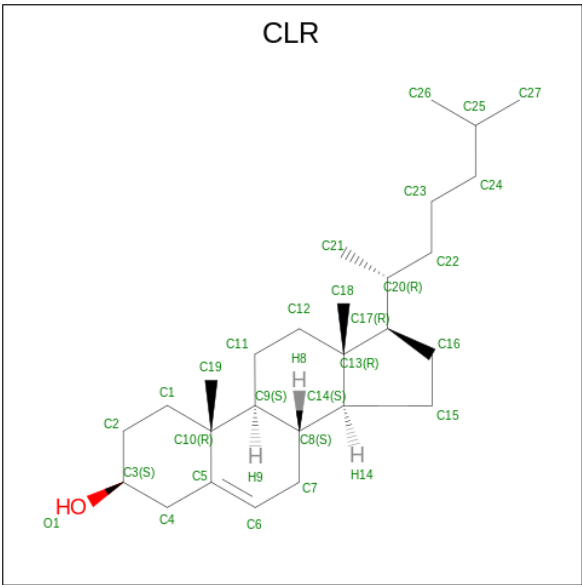
Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	PHE	-	expression tag	UNP Q9Y5N1
R	-2	GLN	-	expression tag	UNP Q9Y5N1
R	-1	GLY	-	expression tag	UNP Q9Y5N1
R	0	PRO	-	expression tag	UNP Q9Y5N1

- Molecule 6 is 4-(1H-imidazol-5-ylmethyl)piperidine (three-letter code: A1LY4) (formula: $C_9H_{15}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	H	N	0
			27	9	15	3	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
7	R	1	74	27	46	1	0

HIS	SER	MET
SER	ALA	PRO
SER	SER	LEU
LEU	LEU	HIS
GLU	GLU	ARG
HIS	LYS	TTR
CYS	ARG	VAL
TRP	MET	GLY
LYS	MET	GLU
	VAL	ALA
	SER	ALA
	GLN	VAL
	S343	GLY
	Q346	ALA
	L360	GLU
	I363	GLY
	W371	ALA
	Y392	GLU
	W393	ALA
	F398	GLY
	L401	GLY
	M404	SER
	S405	VAL
	A406	ALA
	V407	SER
	N408	PRO
	P409	TTR
	V410	SER
	L411	SER
	Y412	GLY
	P413	SER
	L414	SER
	S418	SER
	R421	ARG
	A422	GLY
	F423	TTR
	T424	ARG
	K425	PRO
	L426	GLY
	L427	LEU
	CYS	LYS
	PRO	ARG
	GLN	GLY
	LYS	SER
	LEU	LYS
	LYS	PRO
	ILE	SER
	GLN	ALA
	PRO	SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1LY4, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.90	0/1841	0.66	0/2471
2	B	0.83	0/2654	0.78	0/3597
3	G	0.80	0/450	0.65	0/608
4	S	0.64	0/1839	0.67	0/2493
5	R	0.81	0/2414	0.74	0/3292
All	All	0.80	0/9198	0.72	0/12461

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1811	0	1799	6	0
2	B	2607	0	2510	11	0
3	G	444	0	454	1	0
4	S	1795	0	1727	24	0
5	R	2344	0	2367	40	0
6	R	12	15	0	4	0
7	R	28	46	46	2	0
All	All	9041	61	8903	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.35	1.05
5:R:119:THR:HG23	5:R:206:GLU:HG3	1.36	1.05
2:B:254:ASP:HB2	2:B:261:LEU:CD1	1.99	0.92
4:S:68:PHE:CZ	4:S:83:MET:HE2	2.07	0.89
5:R:412:TYR:HB2	5:R:413:PRO:HD3	1.54	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/354 (62%)	215 (97%)	6 (3%)	0	100	100
2	B	337/358 (94%)	324 (96%)	13 (4%)	0	100	100
3	G	56/71 (79%)	56 (100%)	0	0	100	100
4	S	230/269 (86%)	228 (99%)	2 (1%)	0	100	100
5	R	285/461 (62%)	276 (97%)	9 (3%)	0	100	100
All	All	1129/1513 (75%)	1099 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/305 (66%)	200 (100%)	0	100	100
2	B	282/298 (95%)	280 (99%)	2 (1%)	81	91
3	G	47/58 (81%)	47 (100%)	0	100	100
4	S	198/217 (91%)	198 (100%)	0	100	100
5	R	249/372 (67%)	249 (100%)	0	100	100
All	All	976/1250 (78%)	974 (100%)	2 (0%)	91	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	105	TYR
2	B	234	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1LY4	R	501	-	9,13,13	0.50	0	11,16,16	1.88	2 (18%)
7	CLR	R	502	-	31,31,31	1.21	1 (3%)	48,48,48	1.53	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A1LY4	R	501	-	-	2/3/12/12	1/2/2/2
7	CLR	R	502	-	-	3/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	502	CLR	C16-C17	3.20	1.61	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	A1LY4	C01-C06-C07	3.57	120.24	111.88
6	R	501	A1LY4	C02-C01-C06	-3.51	106.71	112.14
7	R	502	CLR	C12-C11-C9	3.44	119.07	113.11
7	R	502	CLR	C15-C14-C13	3.28	107.79	103.84
7	R	502	CLR	C1-C2-C3	3.07	114.40	110.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	501	A1LY4	C01-C06-C07-C08
7	R	502	CLR	C17-C20-C22-C23
7	R	502	CLR	C21-C20-C22-C23
6	R	501	A1LY4	C05-C06-C07-C08
7	R	502	CLR	C23-C24-C25-C27

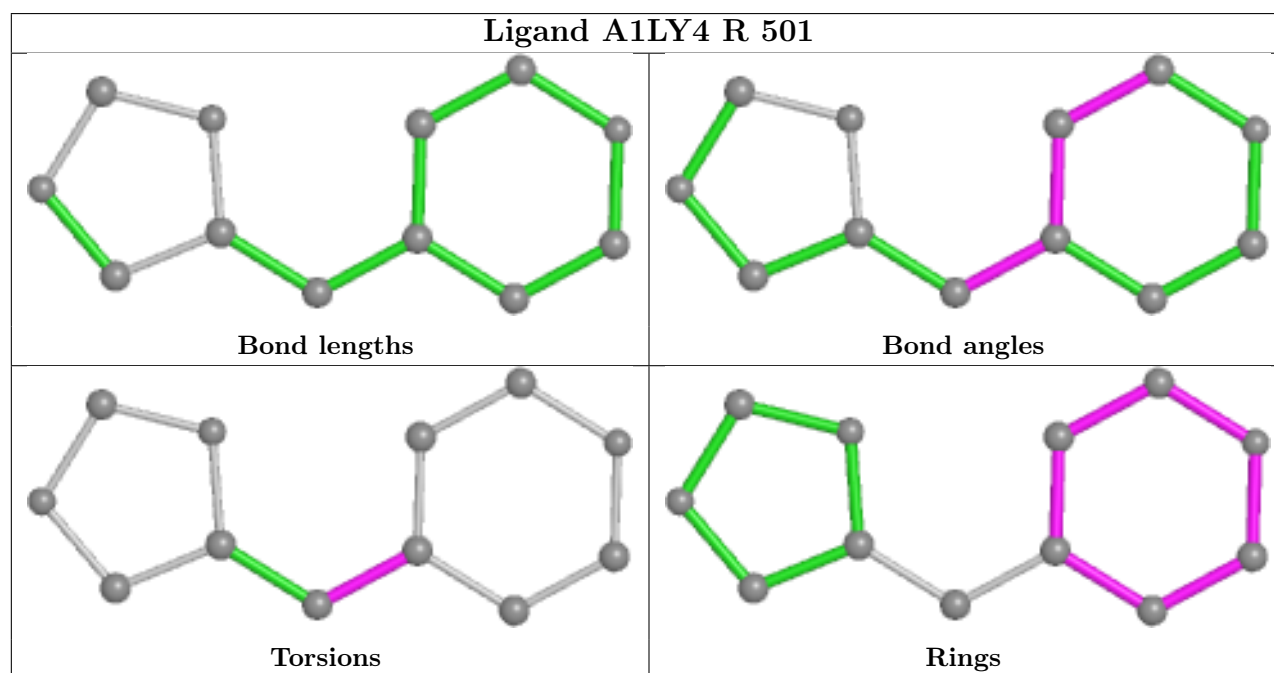
All (1) ring outliers are listed below:

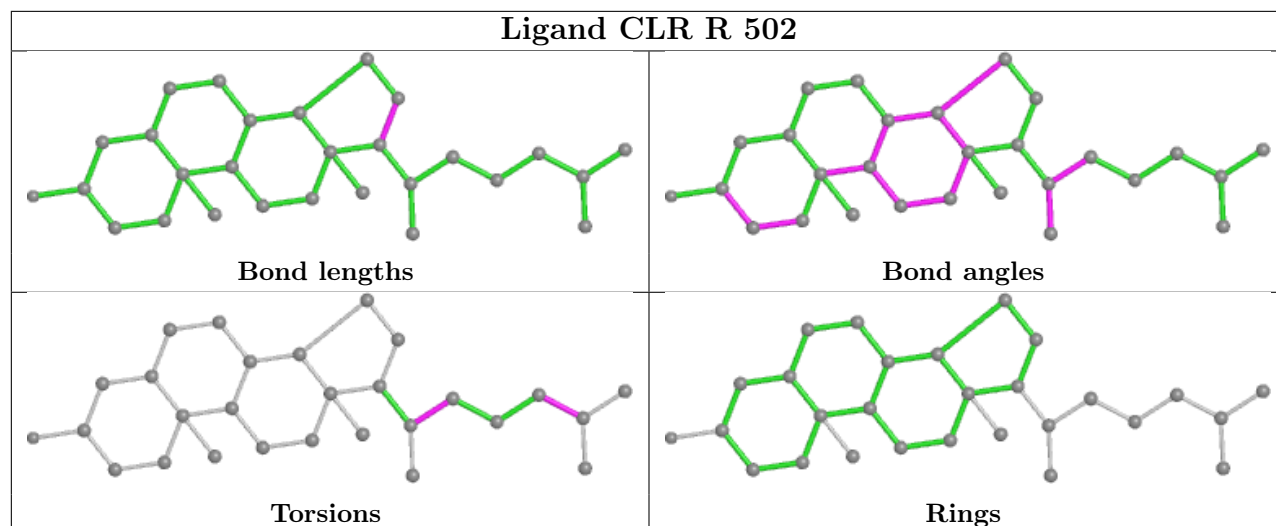
Mol	Chain	Res	Type	Atoms
6	R	501	A1LY4	C01-C02-C04-C05-C06-N03

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	A1LY4	4	0
7	R	502	CLR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.